Urea, (3-methylphenyl)-

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 160 °C

Global applicability domain: Inside

Local applicability domain index: 5.72e-01

Confidence level: 6.35e-01

Nearest Neighbors from the Training Set

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Benzylurea
Measured: 148
Predicted: 152

Image not found

1-Phenylurea
Measured: 147
Predicted: 158

Image not found

Dulcin
Measured: 174
Predicted: 171

Image not found

Ethylphenylacetylurea
Measured: 162
Predicted: 165

Image not found

N-(4-Bromophenyl)urea
Measured: 226
Predicted: 211